

# Chrysene, 1,2,3,4,4a,7,8,9,10,11,12,12a-dodecahydro-6-octyl-

**Other names:** 12-n-Octyl-1,2,3,4,5,6,6a,7,8,9,10,10a-dodecahydrochrysene

**Inchi:** InChI=1S/C26H40/c1-2-3-4-5-6-7-13-21-19-26-22-14-9-8-12-20(22)17-18-25(26)24-16-1

**InchiKey:** QMLSEQMTIVHKQP-UHFFFAOYSA-N

**Formula:** C26H40

**SMILES:** CCCCCCc1cc2c(c3c1CCCC3)CCC1CCCCC21

**Mol. weight [g/mol]:** 352.60

**CAS:** 55281-94-2

## Physical Properties

Property code	Value	Unit	Source
gf	395.59	kJ/mol	Joback Method
hf	-169.06	kJ/mol	Joback Method
hfus	42.61	kJ/mol	Joback Method
hvap	78.96	kJ/mol	Joback Method
log10ws	-9.08		Crippen Method
logp	7.688		Crippen Method
mcvol	320.860	ml/mol	McGowan Method
pc	1153.00	kPa	Joback Method
tb	878.58	K	Joback Method
tc	1099.07	K	Joback Method
tf	506.78	K	Joback Method
vc	1.232	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1097.83	J/molxK	878.58	Joback Method
cpg	1199.56	J/molxK	1062.32	Joback Method
cpg	1181.18	J/molxK	1025.58	Joback Method
cpg	1161.95	J/molxK	988.83	Joback Method
cpg	1141.74	J/molxK	952.08	Joback Method
cpg	1120.41	J/molxK	915.33	Joback Method
cpg	1217.22	J/molxK	1099.07	Joback Method
dvisc	0.0003801	Paxs	878.58	Joback Method

dvisc	0.0004490	Paxs	816.61	Joback Method
dvisc	0.0005450	Paxs	754.65	Joback Method
dvisc	0.0006848	Paxs	692.68	Joback Method
dvisc	0.0009001	Paxs	630.71	Joback Method
dvisc	0.0012557	Paxs	568.75	Joback Method
dvisc	0.0019004	Paxs	506.78	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55281942&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55281942&amp;Units=SI</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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